# Quantization of Hall Conductance in Double Exchange Systems: Topology and Lattice Gauge Field

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We study quantization conditions of the Hall conductivity for a two dimensional system described by a double exchange Hamiltonian with and without an external magnetic field. This is obtained by an extension of the topological arguments familiar from the theory of the integer quantum Hall effect. The quantization conditions are related to spontaneous breaking of spin $O(3)$, time-reversal, and spin chiral symmetries. Extension to systems with higher dimensions is briefly discussed.

The quantum Hall effect (QHE) is a remarkable phenomena in condensed matter physics [1]. After its discovery, there have been many theoretical works which explained the quantization of the Hall conductivity $\sigma_{xy} = n\frac{e^2}{h}$ for two dimensional electron gas in a uniform perpendicular magnetic field. An elegant approach, of which we will make use below, is based on topological and symmetry arguments. For Bloch electrons in a magnetic field, several authors, [2,3] derived an explicit formula for the Hall conductance which is independent on the detailed structure of the periodic potential [4]. The integer $n$ is shown to be a topological invariant, the first Chern class of a $U(1)$ principal fiber bundle on a torus [3]. (See also [5,6].) In a pioneering work by Haldane [7], the possible occurrence of QHE without an external magnetic field in systems with broken time-reversal symmetry and its relation to chiral anomaly in 2d field theories have been discussed. (See also [8].)

The QHE is mainly concerned with charge degrees of freedom of electrons. An experimentally and theoretically relevant question is, therefore, whether there is a similar effect pertaining to the spin degrees of freedom. Indeed, in transition metal oxides, coupling of spin degrees of freedom between itinerant and localized electrons induces many interesting transport properties [9].

In this letter we show that, in principle, a special variant of the QHE may occur also in transition metal oxides with and without an external magnetic field. As we have reported recently [10], the basic ingredients are the Double Exchange (DE) model [11] and the theory developed in Refs. [2,3]. The DE model exhibits rich transport properties [12,9]. The phase factor in the hopping integral [13] induced by the $t_{2g}$ spins leads to an exotic ground state, (referred to as "flux" state), where the Hall conductance is expected to be quantized [10,14]. The mechanism of stabilization of the "flux" state is similar to that of the flux phase discussed in the Hubbard model [15,16] and in a generalized Peierls instability [17]. Numerous other facets due to the Berry phase or to the "flux" were studied, such as an anomalous Hall effect [18,14], Jhan-Teller effect [19], and stripe formation [20].

The conditions we study for the quantization of the Hall conductivity are summarized as follows: (i) the Fermi level should lie in a gap of extended states [2]. (ii) the ground state is not degenerate [2]. (iii) time-reversal symmetry is broken [7]. Condition (iii) is evidently realized in the presence of a uniform external magnetic field in the standard QHE. Alternatively, in the DE model one may perceive two possibilities of breaking time-reversal symmetry: (a) Due to the minimum principle of external flux force line, it is natural to conjecture that the ground state of the DE model has a staggered flux structure [10] where the net spontaneous flux vanishes. However, if a state with non-vanishing spontaneous flux exists, it breaks time-reversal symmetry. The pertinent state is characterized by the Wilson loop [21]. The mechanism of stabilization of such a state was discussed in Refs [18,14]. (b) Even if case (a) is hardly realizable, a system with a proper lattice structure spontaneously breaks the time-reversal symmetry. This kind of symmetry breaking corresponds to that of spin chirality [18,14]. One such example is the Kagome lattice [14]. In the rest of this letter, we first study the Hall conductivity in its general form within the DE model along the lines of TKNN, and then consider some specific examples. Finally, extension to systems with higher dimensions and the relation with theorems due to Lieb [16] and Elitzur [22] are briefly discussed.

The Hamiltonian of the DE model in its minimum version [23] at finite doping reads,

$$H = \sum_{i,j;\mu} \left( -tc^{\dagger}_{i,\mu}c_{j,\mu} + h.c. + J\vec{S}_i \cdot \vec{S}_j \right) - J_H \sum_i \vec{\sigma}_i \cdot \vec{S}_i, \tag{1}$$

where $c_{i,\mu}$ is a fermion (in fact, an $e_g$ electron) annihilation operator at site $i$ with spin projection $\mu$, $\vec{\sigma}$ is the spin operator of the $e_g$ electrons, $\vec{S}_i$ are localized ($t_{2g}$) spins which are treated as classical vectors directed along $(\theta_i, \phi_i)$ in spherical coordinates. Moreover, $J_H$ is the Hund rule coupling constant and $J$ is the direct exchange coupling strength between $t_{2g}$ spins. There is a local $SU(2)$ rotation invariance at every site, and, in the limit $J_H \to \infty$, the original Hamiltonian transforms into [24],

$$\tilde{H} = -t \sum_{\langle i,j \rangle} \left[ \left( \cos\frac{\theta_i}{2}\cos\frac{\theta_j}{2} + e^{-i(\phi_i - \phi_j)}\sin\frac{\theta_i}{2}\sin\frac{\theta_j}{2} \right)c^{\dagger}_i c_j + h.c. \right] + J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j. \tag{2}$$

The current operator on link $ij$ is transformed as

$$v_{ij} = \frac{i}{\hbar}\left(c_i^\dagger c_j - c_j^\dagger c_i\right) \rightarrow \tilde{v}_{ij} = \frac{i}{\hbar}\left[\cos\frac{\theta_i}{2}\cos\frac{\theta_j}{2}\left(c_i^\dagger c_j - c_j^\dagger c_i\right) + \sin\frac{\theta_i}{2}\sin\frac{\theta_j}{2}\left(c_i^\dagger c_j e^{-i(\phi_i-\phi_j)} - c_j^\dagger c_i e^{i(\phi_i-\phi_j)}\right)\right]. \tag{3}$$

The transformation is unitary and does not affect the energy spectrum. However, the link variable which is employed to calculate the Hall conductance is not invariant. Below, we calculate the Hall conductacne, $\sigma_{xy}$, associated with the Hamiltonian (2). The phase factor in the second term in (3) is induced from the $t_{2g}$ spin configuration, which we denote by $\{\theta_i, \phi_i\}$ below. The structure of the phase factor is related to the non-trivial magnetic ordering pattern $\{\theta_i, \phi_i\}$. In a generic configuration, the $e_g$ electron acquires flux which cannot be eliminated by a local gauge transformation, that is, it accumulates a non-zero phase (mod $2\pi$) on moving around a closed path. One of the realizations of this scenario is the "flux" state [10].

We now explain the calculation of $\sigma_{xy}$. In the absence of an external magnetic field, the contribution from the first term in (3) vanishes, so let us concentrate on the second one. (When the field is switched on, the conductivity is the sum of the two terms. The contribution from the first term is obtained within the TKNN formalism.) In the course of its evaluation, one has to employ a Fourier transformation. However, this turn out to be useless since in generic situations, the spin configuration $\{\theta_i, \phi_i\}$ is not periodic. This is due to the property of the DE model where the energy is a functional of the *oriented relative angle* of the $t_{2g}$ spin [10,25]. Thus, for a generic spin configuration, there is no simple algorithm for this calculation problem. Below, we assume a periodicity of the $\{\theta_i, \phi_i\}$ configuration. This can be justified at least for the staggered flux state [10] by noting that the flux state is degenerate. We define the respective unit cells for $\theta$'s and $\phi$'s, $U_\theta$ and $U_\phi$, which are not necessarily identical. These unit cells can be enlarged to the least common multiple (denoted hereafter by $U$) of $U_\theta$ and $U_\phi$, if their ratio is rational. (An interesting situation occurs when the ratio of $U_\theta$ and $U_\phi$ is irrational.)

The expression for the Hall conductivity now reads [3],

$$\sigma_{xy} = \sum_j \left[\frac{e^2}{h}\frac{1}{2\pi i}\oint_{MBZ} d\vec{k}\cdot\langle\vec{k}|\nabla_k|\vec{k}\rangle\right]_j = \frac{e^2}{h}t_r, \tag{4}$$

where $\vec{k}$ is the crystal momentum and $|\vec{k}\rangle$ is a wave function in momentum space defined on the extended magnetic Brillouin zone (MBZ) associated with $U$. Note that here, the MBZ refers to the Brillouin zone of the "spin configuration." Here $j$ is the index of the sub-band. Finally, the number $t_r$ on the right hand side of equation (4) is the solution of the Diophantine equation [2].

The simplest example for which the above formalism can be worked out in detail is the DE model on a square lattice at half-filling. The staggered $\pi$-flux state is spontaneously stabilized [10], and the ground state has an infinite continuous degeneracy. The dispersion relation near the Fermi level is approximated by that for a gapless Dirac fermion. In the absence of an external magnetic field, the time-reversal symmetry is not broken because the spontaneous flux around a plaquette is $\pm\pi$, and the Hall conductance vanishes. Below we assume that the symmetry of the $t_{2g}$ spin is broken, thus removing the continuous degeneracy. We also introduce a next-nearest neighbor (NNN) hopping term for staggered plaquette in order to open an energy gap [26] and to break time-reversal symmetry [7]. We further assume that the staggered structure of the $\pi$-flux in (2) is robust against perturbation by NNN hopping. The effective Hamiltonian for the $e_g$ electron is described by

$$H = -t\sum_{m,n}\left[e^{i\theta_1}c_{m+\frac{1}{2},n+\frac{1}{2}}^\dagger c_{m,n} + e^{i\theta_2}c_{m+\frac{1}{2},n+\frac{1}{2}}^\dagger c_{m+1,n} + e^{i\theta_3}c_{m,n+1}^\dagger c_{m+\frac{1}{2},n+\frac{1}{2}}\right.$$
$$\left.+ e^{i\theta_2}c_{m+1,n+1}^\dagger c_{m+\frac{1}{2},n+\frac{1}{2}} - t'\left(e^{i\theta_4}c_{m,n+1}^\dagger c_{m,n} + e^{i\pi\varphi}c_{m+\frac{1}{2},n+\frac{1}{2}}^\dagger c_{m-\frac{1}{2},n+\frac{1}{2}}\right)\right] + h.c., \tag{5}$$

where $\theta_1 = \pi[\phi(m+\frac{1}{4}) + i2\varphi]$, $\theta_2 = \pi\phi(m+\frac{3}{4})$, $\theta_3 = \pi\phi(m+\frac{1}{4})$, and $\theta_4 = 2\pi\phi m + i\pi\varphi$. Here the effect of the spontaneous staggered $\pi$-flux is replaced by $\varphi = 1/2$. Recently, it has been possible to fabricate networks which are described by the Hamiltonian (5) with $t' = 0$ and to investigate the corresponding energy spectrum [27]. In our calculations, we introduce also a uniform external magnetic field $\phi$ (in the Landau gauge) thus taking into account the experimental setup.

We now derive the Chern number using the method detailed in Ref. [28] which provides a simple counting technique for the TKNN-vortex. In the absence of the external field, i.e. $\phi = 0$, the Hall conductance is quantized as a function of the perturbation, $t_r = sgn(t')$ and $t_r = 0$ for $t' = 0$. The value of $t_r$ for finite $\phi$ is shown in Fig. 1 where the staggered flux state of the DE model can be interpreted only near $\phi \sim 0$.

In the above formalism, we artificially break the time-reversal symmetry and open the energy gap. However, the symmetry would be spontaneously broken away from half-filling because the super-cell structure is expected to stabilize if one employs the analogy between the present model and the generalized Peierls instability [17].

The geometrical structure of the lattice may induce a non-trivial spin configuration [14]. Motivated by the work we study the DE model on a two dimensional pyrochlore like lattice [29], defined by assigning tetrahedrons on the Kagome lattice shared with one of the four triangles (see Fig.2(a)). In the limit $J \to \infty$, the ground state has continuous infinite degeneracy. (Its nature is distinct from that of the Kagome lattice [29] where the relative angle between adjacent spins is $2/3\pi$. In the pyrochlore like lattice, the corresponding angles need not be identical. Typical configurations

are displayed in Fig.2(b)-(e). The spin structure over entire lattice is obtained by combining these tetrahedrons and successively adjusting the relative angles of the shared edges.) Because of the degeneracy, one cannot evaluate (4). Below we assume that one of the spin configurations is selected due to symmetry breaking of the spin and that the periodicity coincides with the Wigner-Seitz cell of the lattice. Employing the method of Ref. [10,25] we optimize the four spin configuration in the Wigner-Seitz cell in order to minimize the kinetic and exchange energies. We studied the model at fillings $x = 1/5, 2/5$, and $3/5$ and confirmed the above picture. Two simple and symmetric realizations are shown in Figs.2(f) and (g). In these examples, the flux through a triangle is exactly $\pi$ and the time-reversal symmetry is not broken. Note that in the degenerate ground state, there exists a spin configuration with broken time-reversal symmetry. An example is shown in Fig.2(e). However, here we study the most extreme cases (f) and (g).

The effective Hamiltonian associated with these states is

$$H = -t \sum_{m,n} \left[ e^{i\frac{2}{3}\pi|\varphi|} c^{\dagger}_{m+1,n} c_{m,n} + e^{-i\frac{2}{3}\pi\varphi} c^{\dagger}_{m,n} c_{m-1,n} + e^{i2\pi m\phi - i\frac{2}{3}\pi|\varphi|} c^{\dagger}_{m,n+1} c_{m,n} + e^{i2\pi m\phi + i\frac{2}{3}\pi\varphi} c^{\dagger}_{m,n} c_{m,n-1} \right.$$
$$+ c^{(1)\dagger}_{m+1,n+1} c_{m,n} + c^{\dagger}_{m,n} c^{(2)}_{m-1,n-1} + e^{i(2m+\frac{1}{3})\pi\phi} c^{(1)\dagger}_{m+1,n+1} c_{m,n+1} + e^{-i(2m-\frac{1}{3})\pi\phi} c^{\dagger}_{m,n-1} c^{(2)}_{m-1,n-1}$$
$$+ e^{i\frac{1}{3}\phi\pi} c^{(1)\dagger}_{m+1,n+1} c_{m+1,n} + e^{-i\frac{1}{3}\phi\pi} c^{\dagger}_{m-1,n} c^{(2)}_{m-1,n-1}$$
$$\left. + e^{i\pi\phi(2m+1) + i\frac{2}{3}\pi|\varphi|} c^{\dagger}_{m,n+1} c_{m+1,n} + e^{i\pi\phi(2m-1) - i\frac{2}{3}\pi\varphi} c^{\dagger}_{m-1,n} c_{m,n-1} \right] + h.c. \tag{6}$$

Here the effect of the spontaneous staggered $\pi$-flux is replaced by $\varphi = \pm 1/2$ for Figs.2(f) and (g), respectively. We also introduce a uniform external magnetic field $\phi$ in the Landau gauge and study the energy gap structure of the model. For a generic $\varphi$, the state shown in Fig.2(f) breaks time-reversal, while the state shown in (g) does not. These two states with different behavior under time reversal are (Kramer) degenerate.

The pertinent Chern number is calculated by using the method developed in Refs. [28,30] where, in the present case, the structure of the complex energy surface is classified as a Riemann surface associated with a ten degree algebraic equation which we have solved numerically. The $t_r$'s are shown in Fig.1(b). The region $\phi \sim 0$ corresponds to the states depicted in Fig.2(f) and (g). Perturbation by additional hopping matrix elements to the honeycomb cell (which is identical to the one discussed in Ref. [7]) opens an energy gap and $\sigma_{xy}$ is quantized to the value associated with the nearest energy gap.

Realizing the quantization conditions (i-iii) is most difficult for the states which we have studied above. Introduction of an anisotropy in the hopping amplitude or exchange energy between in and out of plane bonds induces a tilt from the $\pi$-flux, and the time-reversal symmetry is broken. As another approach, we can construct the entire spin configuration from that of the tetrahedron configuration with broken time-reversal symmetry using the unit shown in Fig.2(e). The occurrence of the QHE in $3d$ pyrochlore was speculated [14]. We confirmed that the energy gap G in Fig. 1(b) survives in $3d$ pyrochlore for an anisotropic inter-layer hopping integral. This leads the QHE in $3d$ [31–33].

*Discussion:* We have investigated the quantization condition of $\sigma_{xy}$ in the ground state of the DE model. In general, it is hard to simultaneously maintain the conditions (i-iii). Especially, the ground state of the DE model have a continuous infinite degeneracy [25] which violates the condition (ii). (The Kramer degeneracy also violates it.) Some different degenerate spin configurations lead the same band structure of the $e_g$ electrons, and the other spin configurations might lead to different band structures. (We denote the Bloch wave associated with the band structures by $|k_i\rangle$ where $i$ is the index of degeneracy.) The full wave function is a superposition of Bloch functions and the integral in equation (4) is ill defined except when all $|k_i\rangle$ have the same Chern number. *Therefore, we should stress that in most cases, the Hall conductance either vanishes or it is ill defined, even when the Fermi energy lies in an energy gap.* The problem associated with this type of degeneracy is not explicitly addressed in TKNN.

On the other hand, the possibility of the quantization cannot be ruled out if symmetry breaking occurs. The *global* spin O(3) symmetry breaking is allowed at zero temperature in $2d$ or at finite temperature in $3d$. The Chern number is different for each spin configuration and the quantized Hall conductivity depends on spin configuration. Therefore, the value of the quantization may serve as a probe determining the spin configuration. (In three or higher dimensions, the QHE occurs [31–33] in transition metal oxides if the system satisfies the conditions (i-iii). For $3d$, each band has three topological invariants (the first Chern numbers) on a 2-tori obtained by slicing the three-torus in three different manners. For general $d$, every quantized invariant on a $d$-dimensional torus $T^d$ is a function of the $d(d-1)/2$ sets of TKNN integers obtained by slicing $T^d$ by the $d(d-1)/2$ distinct $T^2$ [6].)

The DE model with classical spin has *local* symmetry because the ground state energy is a functional of the *oriented relative angles* between spins. The symmetry breaking is difficult. Its relation to the Elitzur's theorem [22] is quite interesting. In this case, the Hall conductance again vanishes or undefined. At least, at half-filling, the $\pi$–flux state is expected to be stabilized in the DE model with quantum spin (even in three dimensions and/or with interactions), because the system maintains reflection positivity in spin space [16].
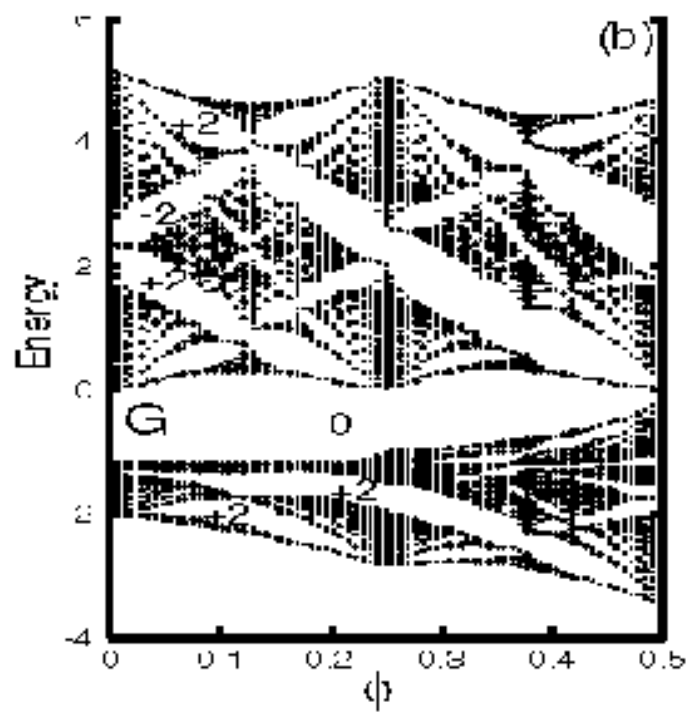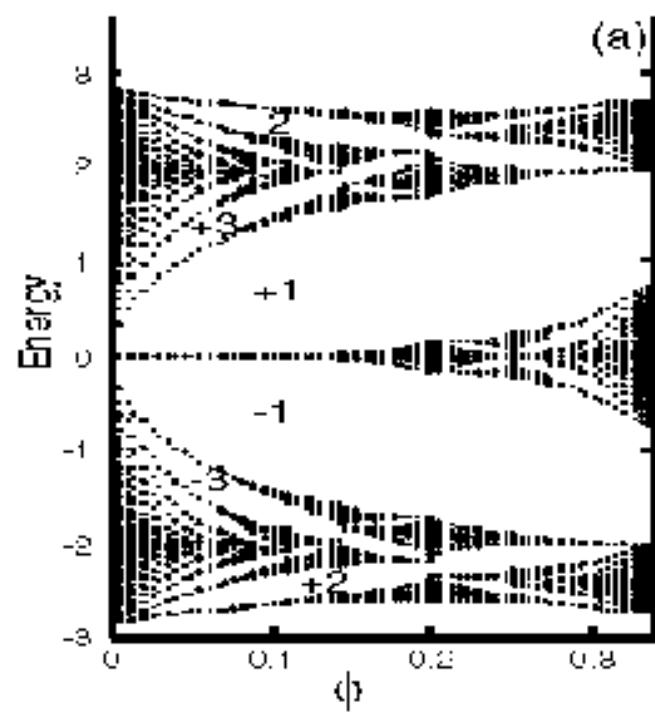
In closing, we point out that flux states in the DE model manifest an interesting physics associated with the QHE and transport properties of transition metal oxides, as well as of networks with modulated nano-structures [27].
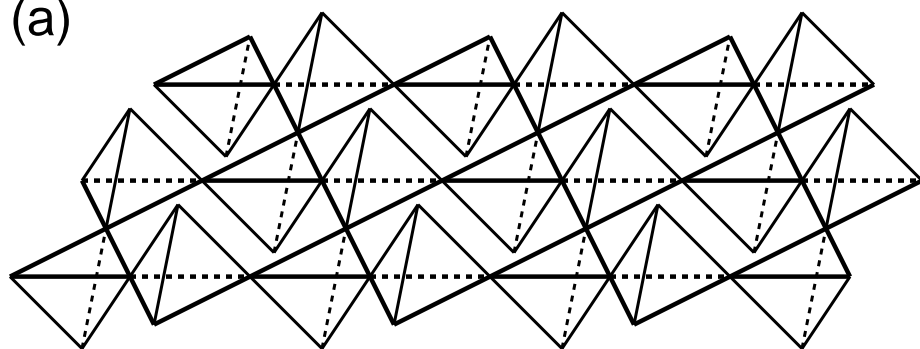
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FIG. 1.    Band structures (a) and (b) as a function of $\phi$ for the Hamiltonians (5) and (6), respectively. Numbers in the energy gaps are $t_r$ in (4).
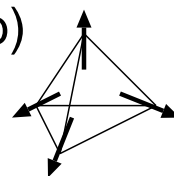
FIG. 2.    (a) Two dimensional pyrochlore like lattice. (b-e) Optimized spin configurations for single tetrahedron cluster in $J \to \infty$. ((b-d) The relative angles are the same and the flux penetrating a triangle is $\pi$. (e) The relative angles are not the same and the flux penetrating a triangle is not $\pi$.) (f) flux configurations constructed from (b) and (c). (g) flux configurations constructed (d), and (b) or (c).
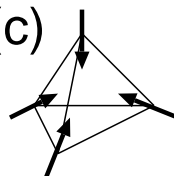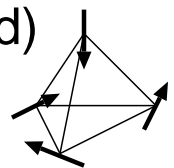
(a)

(b) (c)

(d) (e)

(f)

m-2   m-1   m   m+1   m+2

n+2

n+1

$C_{m+1,n+1}^{(1)}$

$C_{m,n}$

n

$C_{m-1,n-1}^{(2)}$

n-1   $2\varphi$   $2\varphi$

n-2

m   m+1   m+2   m+3

(g)

$\varphi$   $\varphi$   $\varphi$

0   0

$\varphi$   $\varphi$   $\varphi$

0   0   0

$\varphi$   $\varphi$   $\varphi$